

FIG. 6 is a bar representation of the results from sequence independent LGA superpositions. FIG. 6 is Figure 2A in the journal article LGA: a method for finding 3D similarities in protein structures by Adam Zemla, in the journal, Nucleic Acids Research, 2003, Vol. 31, No. 13, pp. 3370-3374.

FIG. 7 shows regions of structural similarity in 3D plot (backbone representation) between the reference structure.

Change(s) applied
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/T.V.R./
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Please replace paragraph [0036] with the replacement paragraph below.

[0036] For given two protein structures the present invention provides a method of finding regions of 3D similarities in protein structures between a first molecule and a second molecule. The method comprises a number of following steps. Comparing the first molecule and the second molecule using Longest Continuous Segments (LCS) analysis. Comparing the first molecule and the second molecule using Global Distance Test (GDT) analysis. Evaluating the calculated alignment between the first molecule and the second molecule using Local Global Alignment Scoring function (LGA_S). For many different alignments repeating the steps above to find the complete set of local and global regions of 3D similarities between given two protein structures. The Local Global Alignment Scoring function (LGA_S) is described in greater detail in the following portions of the DETAILED DESCRIPTION OF THE INVENTION, particularly in paragraph [0036]. The journal article LGA: a method for finding 3D similarities in protein structures by Adam Zemla, in the journal, Nucleic Acids Research, 2003, Vol. 31, No. 13, pp. 3370-3374 includes a section under the heading "Description of the LGA scoring function" which provides additional information about using Local Global Alignment Scoring function (LGA_S). The journal article LGA: a method for finding 3D similarities in protein structures by